

# Optimal Algorithmic Cooling of Spins

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**Abstract.** *Algorithmic Cooling (AC) of Spins* is potentially the first near-future application of quantum computing devices. Straightforward quantum algorithms combined with novel entropy manipulations can result in a method to improve the identification of molecules. We introduce here several new exhaustive cooling algorithms, such as the Tribonacci and  $k$ -bonacci algorithms. In particular, we present the “all-bonacci” algorithm, which appears to reach the maximal degree of cooling obtainable by the optimal AC approach.

## 1 Introduction

Molecules are built from atoms, and the nucleus inside each atom has a property called “spin”. The spin can be understood as the orientation of the nucleus, and when put in a magnetic field, certain spins are binary, either up (ZERO) or down (ONE). Several such bits (inside a single molecule) represent a binary string, or a register. A macroscopic number of such registers/molecules can be manipulated in parallel, as is done, for instance, in Magnetic Resonance Imaging (MRI). The purposes of magnetic resonance methods include the identification of molecules (e.g., proteins), material analysis, and imaging, for chemical or biomedical applications. From the perspective of quantum computation, the spectrometric device that typically monitors and manipulates these bits/spins can be considered a simple “quantum computing” device.

Enhancing the sensitivity of such methods is a Holy Grail in the area of Nuclear Magnetic Resonance (NMR). A common approach to this problem, known as “effective cooling”, has been to reduce the entropy of spins. A spin with lower entropy is considered “cooler” and provides a better signal when used for identifying molecules. To date, effective cooling methods have been plagued by various limitations and feasibility problems.

“Algorithmic Cooling” [1,2,3] is a novel and unconventional effective-cooling method that vastly reduces spin entropy. AC makes use of “data compression” algorithms (that are run on the spins themselves) in combination with “thermalization”. Due to Shannon’s entropy bound (source-coding bound [4]), data compression alone is highly limited in its ability to reduce entropy: the total entropy of the spins in a molecule is preserved, and therefore cooling one spin is done at the expense of heating others. Entropy reduction is boosted dramatically by taking advantage of the phenomenon of thermalization, the natural return of a spins entropy to its thermal equilibrium value where any information encoded on the spin is erased. Our entropy manipulation steps are designed such that the excess entropy is always placed on pre-selected spins, called “reset bits”, which return very quickly to thermal equilibrium. Alternating data compression steps with thermalization of the reset spins thus reduces the total entropy of the spins in the system far beyond Shannon’s bound. The AC of short molecules is experimentally feasible in conventional NMR labs; we, for example, recently cooled spins of a three-bit quantum computer beyond Shannon’s entropy bound [5].

### 1.1 Spin-Temperature and NMR Sensitivity

For two-state systems (e.g. binary spins) there is a simple connection between temperature, entropy, and probability. The difference in probability between the two states is called the *polarization bias*. Consider a single spin particle in a constant magnetic field. At equilibrium with a thermal

heat-bath the probabilities of this spin to be up or down (i.e., parallel or anti-parallel to the magnetic field) are given by:  $p_{\uparrow} = \frac{1+\varepsilon_0}{2}$ , and  $p_{\downarrow} = \frac{1-\varepsilon_0}{2}$ . We refer to a spin as a bit, so that  $|\uparrow\rangle \equiv |0\rangle$  and  $|\downarrow\rangle \equiv |1\rangle$ , where  $|x\rangle$  represents the spin-state  $x$ . The polarization bias is given by  $\varepsilon_0 = p_{\uparrow} - p_{\downarrow} = \tanh\left(\frac{\hbar\gamma B}{2K_B T}\right)$ , where  $B$  is the magnetic field,  $\gamma$  is the particle-dependent gyromagnetic constant,<sup>1</sup>  $K_B$  is Boltzmann's coefficient, and  $T$  is the thermal heat-bath temperature. Let  $\varepsilon = \frac{\hbar\gamma B}{2K_B T}$  such that  $\varepsilon_0 = \tanh \varepsilon$ . For high temperatures or small biases, higher powers of  $\varepsilon$  can be neglected, so we approximate  $\varepsilon_0 \approx \varepsilon$ . Typical values of  $\varepsilon_0$  for nuclear spins (at room temperature and a magnetic field of  $\sim 10$  Tesla) are  $10^{-5} - 10^{-6}$ .

A major challenge in the application of NMR techniques is to enhance sensitivity by overcoming difficulties related to the Signal-to-Noise Ratio (SNR). Five fundamental approaches were traditionally suggested for improving the SNR of NMR. Three straightforward approaches - cooling the entire system, increasing the magnetic field, and using a larger sample - are all expensive and limited in applicability, for instance they are incompatible with live samples. Furthermore, such approaches are often impractical due to sample or hardware limitations. A fourth approach - repeated sampling - is very feasible and is often employed in NMR experiments. However, an improvement of the SNR by a factor of  $M$  requires  $M^2$  repetitions (each followed by a significant delay to allow relaxation), making this approach time-consuming and overly costly. Furthermore, it is inadequate for samples which evolve over the averaged time-scale, for slow-relaxing spins, or for non-Gaussian noise.

## 1.2 Effective cooling of spins

The fifth fundamental approach to the SNR problem consists of cooling the spins without cooling the environment, an approach known as “effective cooling” of the spins [6,7,8,9]. The effectively-cooled spins can be used for spectroscopy until they relax to thermal equilibrium. The following calculations are done to leading order in  $\varepsilon_0$  and are appropriate for  $\varepsilon_0 \ll 1$ . A spin temperature at equilibrium is  $T \propto \varepsilon_0^{-1}$ . The single-spin Shannon entropy is  $H = 1 - (\varepsilon_0^2 / \ln 4)$ . A spin temperature out of thermal equilibrium is similarly defined (see for instance [10]). Therefore, increasing the polarization bias of a spin beyond its equilibrium value is equivalent to cooling the spin (without cooling the system) and to decreasing its entropy.

Several more recent approaches are based on the creation of very high polarizations, for example dynamic nuclear polarization [11], para-hydrogen in two-spin systems [12], and hyperpolarized xenon [13]. In addition, there are other spin-cooling methods, based on general unitary transformations [7] and on (closely related) data compression methods in closed systems [8].

One method for effective cooling of spins, *reversible polarization compression (RPC)*, is based on entropy manipulation techniques. RPC can be used to cool some spins while heating others [7,8]. Contrary to conventional data compression,<sup>2</sup> RPC techniques focus on the low-entropy spins, namely those that get colder during the entropy manipulation process. RPC, also termed “molecular-scale heat engine”, consists of reversible, in-place, lossless, adiabatic entropy manipulations in a closed system [8]. Therefore, RPC is limited by the second law of thermodynamics, which states that entropy in a closed system cannot decrease, as is also stated by Shannon's source coding theorem [4]. Consider the total entropy of  $n$  uncorrelated spins with equal biases,  $H(n) \approx n(1 - \varepsilon_0^2 / \ln 4)$ . This entropy could be compressed into  $m \geq n(1 - \varepsilon^2 / \ln 4)$  high entropy spins, leaving  $n - m$  extremely cold spins with entropy near zero. Due to preservation of entropy, the number of extremely cold spins,  $n - m$ , cannot exceed  $n\varepsilon_0^2 / \ln 4$ . With a typical  $\varepsilon_0 \sim 10^{-5}$ , extremely long molecules ( $\sim 10^{10}$  atoms) are required in order to cool a single spin to a temperature near zero. If we use smaller molecules, with  $n \ll 10^{10}$ , and compress the entropy onto  $n - 1$  fully-random spins, the entropy of the remaining spin satisfies [2]

<sup>1</sup> This constant,  $\gamma$ , is thus responsible for the difference in the equilibrium polarization bias of different spins [e.g., a hydrogen nucleus is about 4 times more polarized than a  $^{13}\text{C}$  nucleus, but less polarized by three orders of magnitude than an electron spin].

<sup>2</sup> Compression of data [4] such as bits in a computer file, can be performed by condensation of entropy to a minimal number of high entropy bits, which are then used as a compressed file.

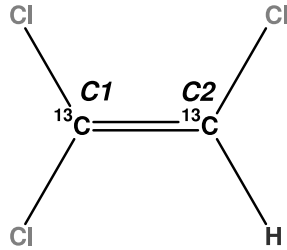
$$1 - \varepsilon_{\text{final}}^2 \geq n(1 - \varepsilon_0^2 / \ln 4) - (n - 1) = 1 - n\varepsilon_0^2 / \ln 4. \quad (1)$$

Thus, the polarization bias of the cooled spin is bounded by

$$\varepsilon_{\text{final}} \leq \varepsilon_0 \sqrt{n}. \quad (2)$$

When all operations are unitary, a stricter bound than imposed by entropy conservation was derived by Sørensen [7]. In practice, due to experimental limitations, such as the efficiency of the algorithm, relaxation times, and off-resonance effects, the obtained cooling is significantly below the bound given in eq 2.

Another effective cooling method is known as *polarization transfer (PT)* [6,14]. This technique may be applied if at thermal equilibrium the spins to be used for spectroscopy (the observed spins) are less polarized than nearby auxiliary spins. In this case, PT from the auxiliary spins to the observed spins is equivalent to cooling the observed spins (while heating the auxiliary spins). PT from one spin to another is limited as a cooling technique, because the polarization bias increase of the observed spin is bounded by the bias of the highly polarized spin. PT is regularly used in NMR spectroscopy, among nuclear spins on the same molecule [6]. As a simple example, consider the 3-bit molecule trichloroethylene (TCE) shown in Fig. 1. The hydrogen nucleus is



**Fig. 1.** A 3-bit computer: a TCE molecule labeled with two  $^{13}\text{C}$ . TCE has three spin nuclei: two carbons and a hydrogen, which are named C1, C2 and H. The chlorines have a very small signal and their coupling with the carbons is averaged out. Therefore, TCE acts as a three-bit computer. The proton can be used as a reset spin because relative to the carbons, its equilibrium bias is four times greater, and its thermalization time is much shorter. Based on the theoretical ideas presented in [2], the hydrogen of TCE was used to cool both carbons, decrease the total entropy of the molecule, and bypass Shannon’s bound on cooling via RPC [5].

about four times more polarized than each of the carbon nuclei; PT from a hydrogen can be used to cool a single carbon by a factor of four. A different form of PT involves shifting entropy from nuclear spins to electron spins. This technique is still under development [9,13], but has significant potential in the future.

Unfortunately, the manipulation of many spins, say  $n > 100$ , is a very difficult task, and the gain of  $\sqrt{n}$  in polarization is not substantial enough to justify putting this technique into practice.

In its most general form, RPC is applied to spins with different initial polarization biases, thus PT is a special case of RPC. We sometimes refer to both techniques and their combination as *reversible algorithmic cooling*.

## 2 Algorithmic Cooling

Boykin, Mor, Roychowdhury, Vatan, and Vrijen (hereinafter referred to as BMRVV), coined the term *Algorithmic Cooling (AC)* for their novel effective-cooling method [1]. AC expands previous effective-cooling techniques by exploiting entropy manipulations in *open systems*. It combines RPC

with relaxation (namely, thermalization) of the *hotter spins*, in order to cool far beyond Shannon’s entropy bound.

AC employs slow-relaxing spins (which we call *computation spins*) and rapidly relaxing spins (*reset spins*), to cool the system by pumping entropy to the environment. Scheme 1 details the three basic operations of AC. The ratio  $R_{\text{relax-times}}$ , between the spin-lattice relaxation times of the computation spins and the reset spins, must satisfy  $R_{\text{relax-times}} \gg 1$ , to permit the application of many cooling steps to the system.

In all the algorithms presented below, we assume that the relaxation time of each computation spin is sufficiently large, so that the entire algorithm is completed before the computation spins lose their polarization.

The practicable algorithmic cooling (PAC) suggested in [2] indicated a potential for near-future application to NMR spectroscopy [3]. In particular, it presented an algorithm (named PAC2) which uses any odd number of spins such that one of them is a reset spin and the other  $2L$  spins are computation spins. PAC2 cools the spins such that the coldest one can (ideally) reach a bias of  $(3/2)^L$ . This proves an exponential advantage of AC over the best possible reversible algorithmic cooling, as reversible cooling techniques (e.g., of refs [7] and [8]) are limited to a bias improvement factor of  $\sqrt{n}$ . As PAC2 can be applied to small  $L$  (and small  $n$ ), it is potentially suitable for near future applications.

**Scheme 1:** AC is based on the combination of three distinct operations:

1. *RPC. Reversible Polarization Compression steps redistribute the entropy in the system so that some computation spins are cooled while other computation spins become hotter than the environment.*
2. *SWAP. Controlled interactions allow the hotter computation spins to adiabatically lose their entropy to a set of reset spins, via PT from the reset spins onto these specific computation spins.*
3. *WAIT. The reset spins rapidly thermalize, conveying their entropy to the environment, while the computation spins remain colder, so that the entire system is cooled.*

## 2.1 Block-Wise Algorithmic Cooling

The original Algorithmic Cooling (BMRVV AC) [1] was designed to address the scaling problem of NMR quantum computing. Thus, a significant number of spins are cooled to a desired level and arranged in a consecutive block, such that the entire block may be viewed as a register of cooled spins. The calculation of the cooling degree attained by the algorithm was based on the law of large numbers, yielding an exponential reduction in spin temperature. Relatively long molecules were required due to this statistical nature, in order to ensure the cooling of 20, 50, or more spins (the algorithm was not analyzed for a small number of spins). All computation spins were assumed to be arranged in a linear chain where each computation spin (e.g.,  $^{13}\text{C}$ ) is attached to a reset spin (e.g.,  $^1\text{H}$ ). Reset and computation spins are assumed to have the same bias  $\varepsilon_0$ . BMRVV AC consists of applying a recursive algorithm repeating (as many times as necessary) the sequence of RPC, SWAP (with reset spins), and WAIT, as detailed in Scheme 1. The relation between gates and NMR pulse sequences is discussed in ref [15].

This cooling algorithm employed a simple form of RPC termed *Basic Compression Subroutine (BCS)* [1]. The computation spins are ordered in pairs, and the following operations are applied to each pair of computation spins  $X, Y$ .  $X_j, Y_j$  denote the state of the respective spin after stage  $j$ ;  $X_0, Y_0$  indicate the initial state.

1. Controlled-NOT (CNOT), with spin  $Y$  as the control and spin  $X$  as target:  $Y_1 = Y_0, X_1 = X_0 \oplus Y_0$ , where  $\oplus$  denotes exclusive OR (namely, addition modulo 2). This means that the target spin is flipped (NOT gate  $|\uparrow\rangle \leftrightarrow |\downarrow\rangle$ ) if the control spin is  $|1\rangle$  (i.e.,  $|\downarrow\rangle$ ). Note that  $X_1 = |0\rangle \Leftrightarrow X_0 = Y_0$ , in which case the bias of spin  $Y$  is doubled, namely the probability that  $Y_1 = |0\rangle$  is very close to  $(1 + 2\varepsilon_0)/2$ .
2. NOT gate on spin  $X_1$ . So  $X_2 = \text{NOT}(X_1)$ .

- Controlled-SWAP (CSWAP), with spin X as a control: if  $X_2 = |1\rangle$  ( $Y$  was cooled), transfer the improved state of  $Y$  (doubled bias) to a chosen location by alternate SWAP and CSWAP gates.

Let us show that indeed in step 1 the bias of spin  $Y$  is doubled whenever  $X_1 = |0\rangle$ . Consider the truth table for the CNOT operation below:

input : $X_0 Y_0$		output : $X_1 Y_1$
0	0	0 0
0	1	1 1
1	0	1 0
1	1	0 1

The probability that both spins are initially  $|0\rangle$  is  $p_{00} \equiv P(X_0 = |0\rangle, Y_0 = |0\rangle) = (1 + \varepsilon_0)^2/4$ . In general,  $p_{kl} \equiv P(X_0 = |k\rangle, Y_0 = |l\rangle)$  such that  $p_{01} = p_{10} = (1 + \varepsilon_0)(1 - \varepsilon_0)/4$ , and  $p_{11} = (1 - \varepsilon_0)^2/4$ . After CNOT, the conditional probability  $P(Y_1 = |0\rangle | X_1 = |0\rangle)$  is  $\frac{q_{00}}{q_{00} + q_{01}} = \frac{p_{00}}{p_{00} + p_{11}}$ , where  $q_{kl} \equiv P(X_1 = |k\rangle, Y_1 = |l\rangle)$  and  $q_{kl}$  is derived from  $p_{kl}$  according to the truth table, so that  $q_{00} = p_{00}$ , and  $q_{01} = p_{11}$ . In terms of  $\varepsilon_0$  this probability is

$$\frac{(1 + \varepsilon_0)^2}{(1 + \varepsilon_0)^2 + (1 - \varepsilon_0)^2} \approx \frac{1 + 2\varepsilon_0}{2},$$

indicating that the bias of  $Y$  was indeed doubled in this case.

For further details regarding the basic compression subroutine and its application to many pairs of spins (in a recursive manner) to reach a bias of  $2^j \varepsilon_0$ , we refer the reader to ref [1].

## 2.2 Practicable Algorithmic Cooling (PAC)

An efficient and experimentally feasible AC technique was later presented, termed “*practicable algorithmic cooling (PAC)*” [2]. Unlike the first algorithm, the analysis of PAC does not rely on the law of large numbers, and no statistical requirement is invoked. PAC is thus a simple algorithm that may be conveniently analyzed, and which is already applicable for molecules containing very few spins. Therefore, PAC has already led to experimental implementations. PAC algorithms use PT steps, reset steps, and *3-bit-compression (3B-Comp)*. As already mentioned, one of the algorithms presented in [2], PAC2, cools the spins such that the coldest one can (ideally) reach a bias of  $(3/2)^L$ , while the number of spins is only  $2L + 1$ . PAC is simple, as all compressions are applied to three spins, often with identical biases. The algorithms we present in the next section are more efficient and lead to a better degree of cooling, but are also more complicated. We believe that PAC is the best candidate for near future applications of AC, such as improving the SNR of biomedical applications.

PAC algorithms [2] use a basic 3-spin RPC step termed 3-bit-compression (3B-Comp):

**Scheme 2:** *3-BitCompression (3BComp)*

- CNOT, with spin B as a control and spin A as a target. Spin A is flipped if  $B = |1\rangle$ .
- NOT on spin A.
- CSWAP with spin A as a control and spins B and C as targets. B and C are swapped if  $A = |1\rangle$ .

Assume that the initial bias of the spins is  $\varepsilon_0$ . The result of scheme 2 is that spin  $C$  is cooled: if  $A = |1\rangle$  after the first step (and  $A = |0\rangle$  after the second step),  $C$  is left unchanged (with its original bias  $\varepsilon_0$ ); if however,  $A = |0\rangle$  after the first step (hence  $A = |1\rangle$  after the second step), spin  $B$  is cooled by a factor of about 2 (see previous subsection), and following the CSWAP the new bias is placed on  $C$ . Therefore, on average,  $C$  is cooled by a factor of 3/2. We do not care about the biases of the other two spins, as they subsequently undergo a reset operation.

In many realistic cases the polarization bias of the reset spins at thermal equilibrium,  $\varepsilon_0$ , is higher than the biases of the computation spins. Thus, an initial PT from reset spins to computation spins (e.g., from hydrogen to carbon or nitrogen), cools the computation spins to the 0<sup>th</sup> purification level,  $\varepsilon_0$ .

As an alternative to Scheme 2, the 3B-Comp operation depicted in Scheme 3 is similar to the CNOT-CSWAP combination (Scheme 2) and cools spin  $C$  to the same degree. This gate is known as the MAJORITY gate since the resulting value of bit  $C$  indicates whether the majority of the bits had values of  $|0\rangle$  or  $|1\rangle$  prior to the operation of the gate.

**Scheme 3:** *Single operation implementing 3B-Comp*

*Exchange the states  $|100\rangle \leftrightarrow |011\rangle$ .*

*Leave the rest of the states unchanged.*

If 3B-Comp is applied to three spins  $\{C, B, A\}$  which have identical biases,  $\varepsilon_C = \varepsilon_B = \varepsilon_A = \varepsilon_0$ , then spin  $C$  will acquire a new bias  $\varepsilon'_C$ . This new bias is obtained from the initial probability that spin  $C$  is  $|0\rangle$  by adding the effect of exchanging  $|100\rangle \leftrightarrow |011\rangle$ :

$$\begin{aligned} \frac{1 + \varepsilon'_C}{2} &= \frac{1 + \varepsilon_C}{2} + p_{|100\rangle} - p_{|011\rangle} \\ &= \frac{1 + \varepsilon_0}{2} + \frac{1 - \varepsilon_0}{2} \frac{1 + \varepsilon_0}{2} \frac{1 + \varepsilon_0}{2} - \frac{1 + \varepsilon_0}{2} \frac{1 - \varepsilon_0}{2} \frac{1 - \varepsilon_0}{2} = \frac{1 + \frac{3\varepsilon_0 - \varepsilon_0^3}{2}}{2}. \end{aligned} \quad (3)$$

The resulting bias is

$$\varepsilon'_C = \frac{3\varepsilon_0 - \varepsilon_0^3}{2}, \quad (4)$$

and in the case where  $\varepsilon_0 \ll 1$

$$\varepsilon'_C \approx \frac{3\varepsilon_0}{2}. \quad (5)$$

We have reviewed two schemes for cooling spin  $C$ : one using CNOT and CSWAP gates (see Scheme 2), and the other using the MAJORITY gate (see Scheme 3). Spin  $C$  reaches the same final bias following both schemes. The other spins may obtain different biases, but this is irrelevant for our purpose, as they undergo a reset operation in the next stages of any cooling algorithm.

The simplest practicable cooling algorithm, termed Practicable Algorithmic Cooling 1 (PAC1) [2], employs dedicated reset spins, which are not involved in compression steps. PAC1 on three computation spins is shown in Fig. 2, where each computation spin  $X$  has a neighboring reset spin,  $r_X$ , with which it can be swapped. The following examples illustrate cooling by PAC1. In order to cool a single spin (say, spin  $C$ ) to the first purification level, start with three computation spins,  $CBA$ , and perform the sequence presented in Example 1.<sup>3</sup>

**Example 1:** *Cooling spin  $C$  to the 1<sup>st</sup> purification level by PAC1*

1.  $PT((r_C \rightarrow C); (r_B \rightarrow B); (r_A \rightarrow A))$ , to initiate all spins.
2.  $3B\text{-}Comp(C; B; A)$ , increase the polarization of  $C$ .

A similar algorithm can also cool the entire molecule beyond Shannon's entropy bound. See the sequence presented in Example 2.

**Example 2:** *Cooling spin  $C$  and bypassing Shannon's entropy bound by PAC1*

1.  $PT((r_C \rightarrow C); (r_B \rightarrow B); (r_A \rightarrow A))$ , to initiate all spins.
2.  $3B\text{-}Comp(C; B; A)$ , increase the polarization of  $C$ .
3. WAIT
4.  $PT((r_B \rightarrow B); (r_A \rightarrow A))$ , to reset spins  $A, B$ .

In order to cool one spin (say, spin  $E$ ) to the second purification level (polarization bias  $\varepsilon_2$ ), start with five computation spins ( $EDCBA$ ) and perform the sequence presented in Example 3.

For small biases, the polarization of spin  $E$  following the sequence in Example 3 is  $\varepsilon_2 \approx (3/2)\varepsilon_1 \approx (3/2)^2\varepsilon_0$ .

**Example 3:** *Cooling spin  $E$  in  $EDCBA$  to the 2nd purification level by PAC1*

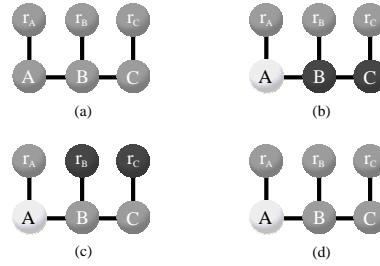
<sup>3</sup> This sequence may be implemented by the application of an appropriate sequence of radiofrequency pulses.

1.  $PT(E; D; C)$ , to initiate spins  $EDC$ .
2.  $3B\text{-}Comp(E; D; C)$ , increase the polarization of  $E$  to  $\varepsilon_1$ .
3. *WAIT*
4.  $PT(D; C; B)$ , to initiate spins  $DCB$ .
5.  $3B\text{-}Comp(D; C; B)$ , increase the polarization of  $D$  to  $\varepsilon_1$ .
6. *WAIT*
7.  $PT(C; B; A)$ , to initiate spins  $CBA$ .
8.  $3B\text{-}Comp(C; B; A)$ , increase the polarization of  $C$  to  $\varepsilon_1$ .
9.  $3B\text{-}Comp(E; D; C)$ , increase the polarization of  $E$  to  $\varepsilon_2$ .

For molecules with more spins, a higher cooling level can be obtained.

This simple practicable cooling algorithm (PAC1) is easily generalized to cool one spin to any purification level  $L$ . [2] The resultant bias will be very close to  $(3/2)^L$ , as long as this bias is much smaller than 1. For a final bias that approaches 1 (close to a pure state), as required for conventional (non-ensemble) quantum computing, a more precise calculation is required.

Consider an array of  $n$  computation spins,  $c_n c_{n-1} \dots c_2 c_1$ , where each computation spin,  $c_i$ , is attached to a reset spin,  $r_i$  (see Fig. 2 for the case of  $n = 3$ ). To cool  $c_k$ , the spin at index  $k$ , to a



**Fig. 2.** An abstract example of a molecule with three computation spins  $A$ ,  $B$  and  $C$ , attached to reset spins  $r_A$ ,  $r_B$ , and  $r_C$ , respectively. All spins have the same equilibrium polarization bias,  $\varepsilon_0$  (a). The temperature after each step is illustrated by color: gray - thermal equilibrium; white - colder than initial temperature; and black - hotter than initial temperature. PAC uses 3-bit compression (3B-Comp), Polarization Transfer (PT) steps, and RESET steps: 1. 3B-Comp( $C; B; A$ ); the outcome of this step is shown in (b). 2.  $PT(r_B \rightarrow B)$ ,  $PT(r_C \rightarrow C)$ ; the outcome is shown in (c). 3. RESET( $r_B, r_C$ ); the outcome is shown in (d). The 3-bit-compression applied in the first step operates on the three computation spins, increasing the bias of spin  $A$  by a factor of  $3/2$ , while heating the other two spins. The 3B-Comp step cools spin  $A$ , and the following PT and RESET steps restore the initial biases of the other spins, thus the entire system is cooled.

purification level  $j \in 1 \dots L$  the procedure  $M_j(k)$  was recursively defined as follows [2]:  $M_0(k)$  is defined as a single PT step from reset spin  $r_k$  to computation spin  $c_k$  to yield a polarization bias of  $\varepsilon_0$  (the 0<sup>th</sup> purification level). The procedure  $M_1(k)$  applies  $M_0$  to the three spins followed by 3B-Comp on these spins, so that spin  $c_k$  is cooled to the first purification level. Similarly,  $M_2(k)$  applies  $M_1$  three times to cool  $c_k; c_{k-1}; c_{k-2}$  to the first purification level, followed by 3B-Comp on these spins, so that spin  $c_k$  is cooled to the second purification level. We use the notation  $\mathcal{B}_{(j-1) \rightarrow j}(k)$  to represent the application of 3B-Comp to spins to purify spin  $c_k$  from  $\varepsilon_{j-1}$  to  $\varepsilon_j$ . Then, the full algorithm has a simple recursive form, described in Algorithm 1.

**Algorithm 1:** *Practicable algorithmic cooling 1 (PAC1):*

For  $j \in \{1, \dots, L\}$

$$M_j(k) = \mathcal{B}_{\{(j-1) \rightarrow j\}}(k) M_{j-1}(k-2) M_{j-1}(k-1) M_{j-1}(k) , \quad (6)$$

applied from right to left ( $M_{j-1}(k)$  is applied first).

For instance,  $M_1(3) = \mathcal{B}_{\{0 \rightarrow 1\}}(3) M_0(1) M_0(2) M_0(3)$ , is 3B-Comp applied after reset as described

in Example 1.<sup>4</sup> Clearly,  $M_1(k)$  can be applied to any  $k \geq 3$ ,  $M_2(k)$  to  $k \geq 5$ , and  $M_j(k)$  to  $k \geq 2j + 1$ . Thus, to cool a single spin to a purification level of  $L$ ,  $2L + 1$  computation spins and an equal number of reset spins are required. A single reset spin could be used for initializing all relevant computation spins, at the expense of additional time steps.

Reset spins may also be used for compression, thus replacing the 3B-Comp and PT steps above by a generalized RPC. The corresponding algorithm, termed PAC2, has an improved space complexity relative to PAC1. We explicitly show how this is achieved. Let  $\varepsilon_0$  be the polarization bias of the reset spin. In order to cool a single spin to  $\varepsilon_1$ , start with two computation spins,  $CB$ , and one reset spin,  $A$ , and perform the sequence shown in Example 4 to cool spin  $C$ .

**Example 4:** *Cooling spin  $C$  to the 1<sup>st</sup> purification level by PAC2*

1.  $PT(A \rightarrow B)$ .
2.  $PT(B \rightarrow C)$  to initiate spin  $C$ .
3.  $RESET(A)$  (by waiting).
4.  $PT(A \rightarrow B)$  to initiate spin  $B$ .
5.  $RESET(A)$ . If the thermalization time of the computation spins is sufficiently large, there are now three spins with polarization bias  $\varepsilon_0$ .
6. 3B-Comp to increase the polarization of spin  $C$  to  $\varepsilon_1$ .

In order to cool one spin (say, spin  $E$ ) to the second purification level (polarization bias  $\varepsilon_2$ ), start with 5 computation spins ( $EDCBA$ ) and follow Example 5.

**Example 5:** *Cooling spin  $E$  in  $EDCBA$  to the 2<sup>nd</sup> purification level by PAC2*

1.  $PT$  sequentially to initiate spins  $EDC$  ( $RESET(A)$  after each  $PT$ ).
2. 3B-Comp on spins  $EDC$  to increase the polarization of spin  $E$  to  $\varepsilon_1$ .
3.  $PT$  sequentially to initiate spins  $DCB$  ( $RESET(A)$  after each  $PT$ ).
4. 3B-Comp on spins  $DCB$  to increase the polarization of spin  $D$  to  $\varepsilon_1$ .
5.  $PT$  sequentially to initiate spins  $CBA$  ( $RESET(A)$  after each  $PT$ ).
6. 3B-Comp on spins  $CBA$  to increase the polarization of spin  $C$  to  $\varepsilon_1$ .
7. 3B-Comp on spins  $EDC$  to increase the polarization of spin  $E$  to  $\varepsilon_2$ .

By repeated application of PAC2 in a recursive manner (as for PAC1), spin systems can be cooled to very low temperatures. PAC1 uses dedicated reset spins, while PAC2 also employs reset spins for compression. The simplest algorithmic cooling can thus be obtained with as few as 3 spins, comprising 2 computation spins and one reset spin.

The algorithms presented so far applied compression steps (3B-Comp) to three identical biases ( $\varepsilon_0$ ); recall that this cools one spin to a new bias,  $\varepsilon'_C \approx (3/2)\varepsilon_0$ . Now consider applying compression to three spins with different biases ( $\varepsilon_C, \varepsilon_B, \varepsilon_A$ ); spin  $C$  will acquire a new bias  $\varepsilon'_C$ , which is a function of the three initial biases [16,17]. This new bias is obtained from the initial probability that spin  $C$  is  $|0\rangle$  by adding the effect of the exchange  $|100\rangle \leftrightarrow |011\rangle$ :

$$\begin{aligned} \frac{1 + \varepsilon'_C}{2} &= \frac{1 + \varepsilon_C}{2} + p_{100} - p_{011} \\ &= \frac{1 + \varepsilon_C}{2} + \frac{1 - \varepsilon_C}{2} \frac{1 + \varepsilon_B}{2} \frac{1 + \varepsilon_A}{2} - \frac{1 + \varepsilon_C}{2} \frac{1 - \varepsilon_B}{2} \frac{1 - \varepsilon_A}{2} \\ &= \frac{1 + \frac{\varepsilon_C + \varepsilon_B + \varepsilon_A - \varepsilon_C \varepsilon_B \varepsilon_A}{2}}{2}. \end{aligned} \quad (7)$$

The resulting bias is

$$\varepsilon'_C = \frac{\varepsilon_C + \varepsilon_B + \varepsilon_A - \varepsilon_C \varepsilon_B \varepsilon_A}{2}, \quad (8)$$

and in the case where  $\varepsilon_C, \varepsilon_B, \varepsilon_A \ll 1$ ,

$$\varepsilon'_C \approx \frac{\varepsilon_C + \varepsilon_B + \varepsilon_A}{2}. \quad (9)$$

---

<sup>4</sup> The procedure of cooling one spin to the second level (starting with five spins) is written as  $M_2(5) = B_{\{1 \rightarrow 2\}}(5) M_1(3) M_1(4) M_1(5)$ .



### 3 Exhaustive Cooling Algorithms

The following examples and derivations are to leading order in the biases. This is justified as long as all biases are much smaller than 1, including the final biases. For example, with  $\varepsilon_0 \sim 10^{-5}$  ( $\varepsilon_0$  is in the order of magnitude of  $10^{-5}$ ) and  $n \leq 13$ , the calculations are fine (see section 4 for details).

#### 3.1 Exhaustive Cooling on Three Spins

**Example 6:** *Fernandez [16]:*  $\mathcal{F}(C, B, A, m)$

*Repeat the following  $m$  times*

1.  $3B\text{-Comp}(C; B; A)$ , to cool  $C$ .
2.  $\text{RESET}(B; A)$

Consider an application of the primitive algorithm in Example 6 to three spins,  $C, B, A$ , where  $A$  and  $B$  are reset spins with initial biases of and (the index over the bias of  $C$  denotes the iteration). After each WAIT step, spins  $A$  and  $B$  are reset back to their equilibrium bias,  $\varepsilon_0$ . As  $B$  and  $A$  play roles of both reset and computation spins, the operation RESET in Example 6 simply means WAIT. From eq 9, after the first iteration

$$\varepsilon_C^{(1)} = \frac{\varepsilon_C^{(0)} + \varepsilon_B + \varepsilon_A}{2} = \frac{0 + 2\varepsilon_0}{2} = \varepsilon_0.$$

After the second iteration

$$\varepsilon_C^{(2)} = \frac{\varepsilon_C^{(1)} + \varepsilon_B + \varepsilon_A}{2} = \frac{\varepsilon_0 + 2\varepsilon_0}{2} = \frac{3\varepsilon_0}{2}.$$

After the  $m^{\text{th}}$  iteration

$$\varepsilon_C^{(m)} = \frac{\varepsilon_C^{(m-1)} + 2\varepsilon_0}{2} = 2^{-m}\varepsilon_C^{(0)} + 2\varepsilon_0 \sum_{j=1}^m 2^{-j} = 0 + (1 - 2^{-m}) 2\varepsilon_0. \quad (10)$$

The asymptotic bias ( $m \rightarrow \infty$ ) may be extracted from

$$\varepsilon_C^{(m)} \approx \frac{\varepsilon_C^{(m)} + 2\varepsilon_0}{2}, \quad (11)$$

with the unique solution and bias configuration

$$\varepsilon_C^{(m)} = 2\varepsilon_0 \Rightarrow \{2\varepsilon_0, \varepsilon_0, \varepsilon_0\}. \quad (12)$$

In order to achieve good asymptotics, one would like to reach  $\varepsilon_C = (2 - \delta)\varepsilon_0$ , where  $\delta$  is arbitrarily small. In this case the number of iterations required is given by  $2^{1-m} = \delta \Rightarrow m = 1 + \lceil \log_2(1/\delta) \rceil$ . For example, if  $\delta = 10^{-5}$ , 18 repetitions are sufficient. Up to an accuracy of  $\delta$ , the biases after the last reset are as in eq 12.

#### 3.2 The Fibonacci Algorithm

An algorithm based on 3B-Comp was recently devised [18], which produces a bias configuration that asymptotically approaches the Fibonacci series. In particular, when applied to  $n$  spins, the coldest spin attains the bias  $\varepsilon_{\text{final}} \approx \varepsilon_0 F_n$ , where  $F_n$  is the  $n^{\text{th}}$  element of the series and  $\varepsilon_0 F_n \ll 1$ . Note that  $\varepsilon_C^{(m)}$  of eq 12 is  $\varepsilon_0 F_3$ . Also note that for 12 spins and  $\varepsilon_0 \sim 10^{-5}$ ,  $\varepsilon_0 F_{12} \ll 1$ , so the approximation is useful for non-trivial spin systems. Compare the bias enhancement factor in this case,  $F_{12} = 144$ , to PAC2 with 13 spins -  $(3/2)^6 \approx 11$ .

Example 7 expands Example 6 to four spins with initial biases  $\varepsilon_D = \varepsilon_C = 0$  and  $\varepsilon_B = \varepsilon_A = \varepsilon_0$  ( $A, B$  are reset spins). We refer to the parameter  $m$  from Example 6 as  $m_3$ , the number of repetitions applied to three spins. We refer to  $\mathcal{F}$  from Example 6 as  $\mathcal{F}_2$  for consistency with the rest of the section. Consider the following example:

**Example 7:**  $\mathcal{F}_2(D, C, B, A, m_4, m_3)$

Repeat the following  $m_4$  times:

1.  $3B\text{-Comp}(D; C; B)$ , places the new bias on spin  $D$ .
2.  $\mathcal{F}_2(C, B, A, m_3)$ .

After each iteration,  $i$ , the bias configuration is  $\{\varepsilon_D^{(i)}, \varepsilon_C^{m_3}, \varepsilon_0, \varepsilon_0\}$ . Running the two steps in Example 7 exhaustively ( $m_4, m_3 \gg 1$ ) yields:

$$\begin{aligned}\varepsilon_C^{(m_3)} &\approx 2\varepsilon_0, \\ \varepsilon_D^{(m_4)} &\approx \frac{\varepsilon_B + \varepsilon_C^{(m_3)} + \varepsilon_D^{(m_4)}}{2} \\ &\Rightarrow \varepsilon_D^{(m_4)} = \varepsilon_B + \varepsilon_C^{(m_3)} = 3\varepsilon_0 = \varepsilon_0 F_4.\end{aligned}\tag{13}$$

This unique solution was obtained by following the logic of eqs 11 and 12.

We generalize this algorithm to  $n$  spins  $A_n, \dots, A_1$  in Algorithm 2.

**Algorithm 2:** *Fibonacci*  $\mathcal{F}_2(A_n, \dots, A_1, m_n, m_3)$

Repeat the following  $m_n$  times:

1.  $3B\text{-Comp}(A_n; A_{n-1}; A_{n-2})$ .
2.  $\mathcal{F}_2(A_{n-1}, \dots, A_1, m_{n-1}, \dots, m_3)$ .

[with  $\mathcal{F}_2(A_3, A_2, A_1, m_3)$  defined by Example 6.]

Note that different values of  $m_{n-1}, \dots, m_3$  may be applied at each repetition of step 2 in Algorithm 2. This is a recursive algorithm; it calls itself with one less spin. Running Algorithm 2 exhaustively ( $m_n, m_{n-1}, \dots, m_3 \gg 1$ ) results, similarly to eq 13, in

$$\begin{aligned}\varepsilon_{A_n}^{(m_n)} &\approx \frac{\varepsilon_{A_n}^{(m_n)} + \varepsilon_{A_{n-1}} + \varepsilon_{A_{n-2}}}{2} \\ &\Rightarrow \varepsilon_{A_n}^{(m_n)} \approx \varepsilon_{A_{n-1}} + \varepsilon_{A_{n-2}}.\end{aligned}\tag{14}$$

This formula yields the Fibonacci series  $\{\dots, 8, 5, 3, 2, 1, 1\}$ , therefore  $\varepsilon_{A_i} \rightarrow \varepsilon_0 F_i$ . We next devise generalized algorithms which achieve better cooling. An analysis of the time requirements of the Fibonacci cooling algorithm is provided in [18].

### 3.3 The Tribonacci Algorithm

Consider 4-bit-compression (4B-Comp) which consists of an exchange between the states  $|1000\rangle$  and  $|0111\rangle$  (the other states remain invariant similar to 3B-Comp). Application of 4B-Comp to four spins  $D, C, B, A$  with corresponding biases  $\varepsilon_D, \varepsilon_C, \varepsilon_B, \varepsilon_A \ll 1$  results in a spin with the probability of the state  $|0\rangle$  given by

$$\frac{1 + \varepsilon'_D}{2} = \frac{1 + \varepsilon_D}{2} + p_{|1000\rangle} - p_{|0111\rangle} \approx \frac{1 + \frac{\varepsilon_A + \varepsilon_B + \varepsilon_C + 3\varepsilon_D}{4}}{2},\tag{15}$$

following the logic of eqs 7 and 8, and finally

$$\varepsilon'_D \approx (\varepsilon_A + \varepsilon_B + \varepsilon_C + 3\varepsilon_D)/4.\tag{16}$$

Example 8 applies an algorithm based on 4B-Comp to 4 spins, with initial biases  $\varepsilon_D = \varepsilon_C = 0$  ( $A, B$  are reset spins). In every iteration of Example 8, running step 2 exhaustively yields the following biases:  $\varepsilon_C = 2\varepsilon_0, \varepsilon_B = \varepsilon_A = \varepsilon_0$ . The compression step (step 1) is then applied onto the configuration

**Example 8:**  $\mathcal{F}_3(D, C, B, A, m_4, m_3)$

Repeat the following  $m_4$  times:

1.  $4B\text{-Comp}(D; C; B; A)$ .
2.  $\mathcal{F}_2(C, B, A, m_3)$ .

From eq 16,  $\varepsilon_D^{(i+1)} = (4\varepsilon_0 + 3\varepsilon_D^{(i)})/4$ . For sufficiently large  $m_4$  and  $m_3$  the algorithm produces final polarizations of

$$\varepsilon_D^{(m_4)} \approx \varepsilon_0 + \frac{3}{4}\varepsilon_D^{(m_4)} \implies \varepsilon_D^{(m_4)} \approx 4\varepsilon_0. \quad (17)$$

For more than 4 spins, a similar 4B-Comp based algorithm may be defined. Example 9 applies an algorithm based on 4B-Comp to 5 spins.

**Example 9:**  $\mathcal{F}_3(E, D, C, B, A, m_5, m_4, m_3)$

Repeat the following  $m_5$  times:

1.  $4B\text{-Comp}(E; D; C; B)$ .
2.  $\mathcal{F}_3(D, C, B, A, m_4, m_3)$ .

Step 2 is run exhaustively in each iteration; the biases of  $DCBA$  after this step are  $\varepsilon_D = 4\varepsilon_0, \varepsilon_C = 2\varepsilon_0, B = A = \varepsilon_0$ . The 4B-Comp step is then applied to the biases of spins  $(E, D, C, B)$ . Similarly to eq 16,  $\varepsilon_E^{(i+1)} = (7\varepsilon_0 + 3\varepsilon_E^{(i)})/4$ . Hence, for sufficiently large  $m_5$  and  $m_4$  the final bias of  $E$  is

$$\varepsilon_E^{(m_5)} \approx (7\varepsilon_0 + 3\varepsilon_E^{(m_5)})/4 \Rightarrow \varepsilon_E^{(m_5)} \approx 7\varepsilon_0. \quad (18)$$

Algorithm 3 applies to an arbitrary number of spins  $n > 4$ . This is a recursive algorithm, which calls itself with one less spin.

**Algorithm 3:** *Tribonacci:*  $\mathcal{F}_3(A_n, \dots, A_1, m_n, \dots, m_3)$

Repeat the following  $m_n$  times:

1.  $4B\text{-Comp}(A_n; A_{n-1}; A_{n-2}; A_{n-3})$ .
2.  $\mathcal{F}_3(A_{n-1}, \dots, A_1, m_{n-1}, \dots, m_3)$ .

[With  $\mathcal{F}_3(A_4, A_3, A_2, A_1, m_4, m_3)$  given by Example 8.]

The compression step, 4B-Comp, is applied to

$$\varepsilon_{A_n}^{(i)}, \varepsilon_{A_{n-1}}, \varepsilon_{A_{n-2}}, \varepsilon_{A_{n-3}},$$

and results in

$$\varepsilon_{A_n}^{(i+1)} = (\varepsilon_{A_{n-1}} + \varepsilon_{A_{n-2}} + \varepsilon_{A_{n-3}} + 3\varepsilon_{A_n}^{(i)})/4. \quad (19)$$

For sufficiently large  $m_j, j = 3, \dots, n$

$$\begin{aligned} \varepsilon_{A_n}^{(m_n)} &\approx (\varepsilon_{A_{n-1}} + \varepsilon_{A_{n-2}} + \varepsilon_{A_{n-3}} + 3\varepsilon_{A_n}^{(m_n)})/4 \\ &\Rightarrow \varepsilon_{A_n}^{(m_n)} \approx \varepsilon_{A_{n-1}} + \varepsilon_{A_{n-2}} + \varepsilon_{A_{n-3}}. \end{aligned} \quad (20)$$

For  $\varepsilon_{A_3} = 2\varepsilon_0, \varepsilon_{A_2} = \varepsilon_{A_1} = \varepsilon_0$ , the resulting bias will be  $\varepsilon_{A_n}^{(m_n)} \approx \varepsilon_0 T_n$ , where  $T_n$  is the  $n^{\text{th}}$  Tribonacci number.<sup>5</sup> As for the Fibonacci algorithm, we assume  $\varepsilon_0 T_n \ll 1$ . The resulting series is  $\{\dots, 24, 13, 7, 4, 2, 1, 1\}$ .

### 3.4 The $k$ -bonacci Algorithm

A direct generalization of the Fibonacci and Tribonacci algorithms above is achieved by the application of  $(k+1)$ -bit-compression, or  $(k+1)\text{B-Comp}$ . This compression on  $k+1$  spins involves the exchange of  $|100\dots 000\rangle$  and  $|011\dots 111\rangle$ , leaving the other states unchanged. When  $(k+1)\text{B-Comp}$  is applied to  $k+1$  spins with biases  $\{\varepsilon_{A_{k+1}}, \varepsilon_{A_k}, \dots, \varepsilon_{A_2}, \varepsilon_{A_1}\}$ , where  $A_1$  and  $A_2$  are reset spins, the probability that the leftmost spin is  $|0\rangle$  becomes (similarly to eq 15)

$$\frac{1 + \varepsilon'_{k+1}}{2} = \frac{1 + \varepsilon_{k+1}}{2} + p_{100\dots 000} - p_{011\dots 111} \approx \frac{1 + \frac{(2^{k-1}-1)\varepsilon_{A_{k+1}} + \sum_{j=1}^k \varepsilon_{A_j}}{2^{k-1}}}{2}. \quad (21)$$

<sup>5</sup> The Tribonacci series (also known as the Fibonacci 3-step series) is generated by the recursive formula  $a_i = a_{i-1} + a_{i-2} + a_{i-3}$ , where  $a_3 = 2$  and  $a_2 = a_1 = 1$ .

Therefore, the bias of the leftmost spin becomes

$$\varepsilon'_{k+1} \approx \frac{(2^{k-1} - 1)\varepsilon_{A_{k+1}} + \sum_{j=1}^k \varepsilon_{A_j}}{2^{k-1}}. \quad (22)$$

Example 10 applies an algorithm based on  $(k+1)$ B-Comp to  $k+1$  spins.  $\mathcal{F}_k$  on  $k+1$  spins calls (recursively)  $\mathcal{F}_k - 1$  on  $k$  spins (recall that  $F_3$  on four spins called  $F_2$  on three spins).

**Example 10:**  $\mathcal{F}_k(A_{k+1}, \dots, A_1, m_{k+1}, \dots, m_3)$

repeat the following  $m_{k+1}$  times:

1.  $(k+1)$ B-Comp( $A_{k+1}, A_k, \dots, A_2, A_1$ )
2.  $\mathcal{F}_{k-1}(A_k, \dots, A_1, m_k, \dots, m_3)$

If step 2 is run exhaustively at each iteration, the resulting biases are

$$\varepsilon_{A_k} = 2^{k-2}\varepsilon_0, \varepsilon_{A_{k-1}} = 2^{k-3}\varepsilon_0, \dots, \varepsilon_{A_3} = 2\varepsilon_0, \varepsilon_{A_2} = \varepsilon_{A_1} = \varepsilon_0.$$

The  $(k+1)$ B-Comp step is then applied to the biases  $\varepsilon_{A_{k+1}}^{(i)}, 2^{k-2}\varepsilon_0, 2^{k-3}\varepsilon_0, \dots, 2\varepsilon_0, \varepsilon_0, \varepsilon_0$ . From eq 22,

$$\varepsilon_{A_{k+1}}^{(i+1)} \approx \frac{(2^{k-1} - 1)\varepsilon_{A_{k+1}}^{(i)} + 2^{k-1}\varepsilon_0}{2^{k-1}}.$$

Hence, for sufficiently large  $m_j, j = 3, \dots, k+1$ , the final bias of  $A_{k+1}$  is

$$\varepsilon_{A_{k+1}}^{(m_{k+1})} \approx \frac{(2^{k-1} - 1)\varepsilon_{A_{k+1}}^{(m_{k+1})} + 2^{k-1}\varepsilon_0}{2^{k-1}} \Rightarrow \varepsilon_{A_{k+1}}^{(m_{k+1})} \approx 2^{k-1}\varepsilon_0. \quad (23)$$

For more than  $k+1$  spins a similar  $(k+1)$ B-Comp based algorithm may be defined. Example 11 applies such an algorithm to  $k+2$  spins.

**Example 11:**  $\mathcal{F}_k(A_{k+2}, \dots, A_1, m_{k+2}, \dots, m_3)$

Repeat the following steps  $m_{k+2}$  times:

1.  $(k+1)$ B-Comp( $A_{k+2}, A_{k+1}, \dots, A_3, A_2$ )
2.  $\mathcal{F}_k(A_{k+1}, \dots, A_1, m_{k+1}, \dots, m_3)$  [defined in Example 11.]

When step 2 is run exhaustively at each iteration, the resulting biases are

$$\varepsilon_{A_{k+1}} = 2^{k-1}\varepsilon_0, \varepsilon_{A_k} = 2^{k-2}\varepsilon_0, \dots, \varepsilon_{A_3} = 2\varepsilon_0, \varepsilon_{A_2} = \varepsilon_{A_1} = \varepsilon_0.$$

The  $(k+1)$ B-Comp is applied to the biases. From Eq. 22,

$$\varepsilon_{A_{k+2}}^{(i+1)} = \frac{(2^{k-1} - 1)\varepsilon_{A_{k+2}}^{(i)} + (2^k - 1)\varepsilon_0}{2^{k-1}}.$$

Hence, for sufficiently large  $m_j, j = 3, \dots, k+2$ , the final bias of  $A_{k+2}$  is

$$\varepsilon_{A_{k+2}}^{(m_{k+2})} \approx \frac{(2^{k-1} - 1)\varepsilon_{A_{k+2}}^{(m_{k+2})} + (2^k - 1)\varepsilon_0}{2^{k-1}} \Rightarrow \varepsilon_{A_{k+2}}^{(m_{k+2})} \approx (2^k - 1)\varepsilon_0. \quad (24)$$

Algorithm 4 generalizes Examples 10 and 11.

**Algorithm 4:**  $k$ -bonacci:  $\mathcal{F}_k(A_n, \dots, A_1, m_n, \dots, m_3)$

Repeat the following  $m_n$  times:

1.  $(k+1)$ B-Comp( $A_n, A_{n-1}, \dots, A_{n-k}$ ).
2.  $\mathcal{F}_k(A_{n-1}, \dots, A_1, m_{n-1}, \dots, m_3)$ .

[with  $\mathcal{F}_k(A_{k+1}, \dots, A_1, m_{k+1}, \dots, m_3)$  defined in Example 10.]

The algorithm is recursive; it calls itself with one less spin. The compression step,  $(k+1)$ B-Comp, is applied to

$$\varepsilon_{A_n}^{(i)}, \varepsilon_{A_{n-1}}, \dots, \varepsilon_{A_{n-k}}.$$

From Eq. 22, the compression results in

$$\varepsilon_{A_n}^{(i+1)} \approx \frac{(2^{k-1} - 1)\varepsilon_{A_n}^{(i)} + \sum_{j=1}^k \varepsilon_{A_{n-j}}}{2^{k-1}}. \quad (25)$$

For sufficiently large  $m_n, m_{n-1}$ , etc.

$$\begin{aligned} \varepsilon_{A_n}^{(m_n)} &\approx \frac{(2^{k-1} - 1)\varepsilon_{A_n}^{(m_n)} + \sum_{j=1}^k \varepsilon_{A_{n-j}}}{2^{k-1}} \\ \Rightarrow \varepsilon_{A_n}^{(m_n)} &\approx \sum_{j=1}^k \varepsilon_{A_{n-j}} \end{aligned} \quad (26)$$

This set of biases corresponds to the  $k$ -step Fibonacci sequence which is generated by a recursive formula.

$$a_1, a_2 = 1, a_\ell = \begin{cases} \sum_{i=1}^{\ell-1} a_{\ell-i}, & 3 \leq \ell \leq k+1 \\ \sum_{i=1}^k a_{\ell-i} & \ell > k+1 \end{cases}. \quad (27)$$

Notice that for  $3 \leq \ell \leq k+1$ ,

$$a_\ell = \sum_{i=1}^{\ell-1} a_i = 1 + 1 + 2 + 4 + \dots + 2^{\ell-4} + 2^{\ell-3} = 2^{\ell-2}. \quad (28)$$

The algorithm uses  $\ell$ -bit-compression ( $\ell$ -B-Comp) gates, where  $3 \leq \ell \leq k+1$ .

### 3.5 The All-bonacci Algorithm

In Example 11 ( $\mathcal{F}_k$  applied to  $k+1$  spins), the resulting biases of the computation spins,  $2^{k-1}\varepsilon_0, 2^{k-2}\varepsilon_0, \dots, 2\varepsilon_0, \varepsilon_0$ , were proportional to the exponential series  $\{2_{k-1}, 2_{k-2}, \dots, 4, 2, 1\}$ . For example,  $\mathcal{F}_2$  on 3 spins results in  $\{2\varepsilon_0, \varepsilon_0, \varepsilon_0\}$  (see Example 6), and  $\mathcal{F}_3$  on 4 spins results in  $\{4\varepsilon_0, 2\varepsilon_0, \varepsilon_0, \varepsilon_0\}$  (see Example 8). This coincides with the  $k$ -step Fibonacci sequence, where  $a_\ell = 2^{\ell-2}$ , for  $a_1 = 1$  and  $\ell = 2, 3, \dots, k+1$  (see eq 28). This property leads to cooling of  $n+1$  spins by a special case of  $k$ -bonacci (Algorithm 5), where  $k$ -bonacci is applied to  $k = n-1$  spins.

**Algorithm 5:** *All-bonacci:*  $\mathcal{F}_{\text{All}}(A_n, \dots, A_1, m_n, \dots, m_3)$

*Apply*  $\mathcal{F}_{n-1}(A_n, \dots, A_1, m_n, \dots, m_3)$ .

The final biases after all-bonacci are  $\varepsilon_{A_i} \rightarrow \varepsilon_0 2^{i-2}$  for  $i > 1$ . The resulting series is  $\{\dots, 16, 8, 4, 2, 1, 1\}$ .

The all-bonacci algorithm potentially constitutes an optimal AC scheme, as explained in section 4.

### 3.6 Density Matrices of the Cooled Spin Systems

For a system of three spins in a completely mixed state (CMS), the density matrix of each spin is For a spin system in a completely mixed state, the density matrix of each spin is:

$$\frac{1}{2}\mathcal{I} = \frac{1}{2} \begin{pmatrix} 1 & \\ & 1 \end{pmatrix}. \quad (29)$$

The density matrix of the entire system, which is diagonal, is given by the tensor product  $\rho_{CM} = \frac{1}{2^3}\mathcal{I} \otimes \mathcal{I} \otimes \mathcal{I}$ , where

$$\text{Diag}(\rho_{CM}) = 2^{-3}(1, 1, 1, 1, 1, 1, 1, 1). \quad (30)$$

For three spins in a thermal state, the density matrix of each spin is

$$\rho_T^{(1)} = \frac{1}{2} \begin{pmatrix} 1 + \varepsilon_0 & \\ & 1 - \varepsilon_0 \end{pmatrix}. \quad (31)$$

and the density matrix of the entire system is given by the tensor product  $\rho_T = \rho_T^{(1)} \otimes \rho_T^{(1)} \otimes \rho_T^{(1)}$ . This matrix is also diagonal. We write the diagonal elements to leading order in  $\varepsilon_0$ :

$$\text{Diag}(\rho_T) = 2^{-3}(1 + 3\varepsilon_0, 1 + \varepsilon_0, 1 + \varepsilon_0, 1 + \varepsilon_0, 1 - \varepsilon_0, 1 - \varepsilon_0, 1 - \varepsilon_0, 1 - 3\varepsilon_0). \quad (32)$$

Consider now the density matrix after shifting and scaling,  $\rho' = 2^n(\rho - 2^{-n}\mathcal{I})/\varepsilon_0$ . For any  $\text{Diag}(\rho) = (p_1, p_2, p_3, \dots, p_n)$  the resulting diagonal is  $\text{Diag}(\rho') = (p'_1, p'_2, p'_3, \dots, p'_n)$  with  $p'_j = 2^n(p_j - 2^{-n})/\varepsilon_0$ . The diagonal of a shifted and scaled (S&S) matrix for a completely mixed state (eq 30) is

$$\text{Diag}(\rho'_{CM}) = (0, 0, 0, 0, 0, 0, 0, 0), \quad (33)$$

and for a thermal state (eq. 32)

$$\text{Diag}(\rho'_T) = (3, 1, 1, 1, -1, -1, -1, -3). \quad (34)$$

In the following discussion we assume that any element,  $p$ , satisfies  $p'\varepsilon_0 \ll 1$ . When applied to a diagonal matrix with elements of the form  $p = \frac{1}{2^n}(1 \pm p'_i\varepsilon_0)$ , this transformation yields the corresponding S&S elements,  $\pm p'i$ .

Consider now the application of the Fibonacci to three spins. The resultant bias configuration,  $\{2\varepsilon_0, \varepsilon_0, \varepsilon_0\}$  (eq 12) is associated with the density matrix

$$\rho_{Fib}^{(3)} = \frac{1}{2^3} \begin{pmatrix} 1 + 2\varepsilon_0 & \\ & 1 - 2\varepsilon_0 \end{pmatrix} \otimes \begin{pmatrix} 1 + \varepsilon_0 & \\ & 1 - \varepsilon_0 \end{pmatrix} \otimes \begin{pmatrix} 1 + \varepsilon_0 & \\ & 1 - \varepsilon_0 \end{pmatrix}, \quad (35)$$

with a corresponding diagonal, to leading order in  $\varepsilon_0$ ,

$$\text{Diag}(\rho_{Fib}^{(3)}) = 2^{-3}(1 + 4\varepsilon_0, 1 + 2\varepsilon_0, 1 + 2\varepsilon_0, 1, 1, 1 - 2\varepsilon_0, 1 - 2\varepsilon_0, 1 - 4\varepsilon_0). \quad (36)$$

The S&S form of this diagonal is

$$\text{Diag}(\rho'_{Fib}^{(3)}) = (4, 2, 2, 0, 0, -2, -2, -4). \quad (37)$$

Similarly, the S&S diagonal for Tribonacci on four spins is

$$\text{Diag}(\rho'_{Trib}^{(4)}) = (8, 6, 6, 4, 4, 2, 2, 0, 0, -2, -2, -4, -4, -6, -6, -8). \quad (38)$$

and the S&S form of the diagonal for all-bonacci on  $n$  spins is

$$\text{Diag}(\rho'_{allb}^{(n)}) = [2^{n-1}, (2^{n-1} - 2), (2^{n-1} - 2), \dots, 2, 2, 0, 0, \dots, -2^n + 1]. \quad (39)$$

which are good approximations as long as  $2^n\varepsilon_0 \ll 1$ .

**Partner Pairing Algorithm** Recently a cooling algorithm was devised that achieves a superior bias than previous AC algorithms. [18,19] This algorithm, termed the Partner Pairing Algorithm (PPA), was shown to produce the highest possible bias for an arbitrary number of spins after any number of reset steps. Let us assume that the reset spin is the least significant bit (the rightmost spin in the tensor-product density matrix). The PPA on  $n$  spins is given in Algorithm 6.

**Algorithm 6:** *Partner Pairing Algorithm (PPA)*

*Repeat the following, until cooling arbitrarily close to the limit.*

1. *RESET* – applied only to a single reset spin.

2. *SORT* – A permutation that sorts the  $2^n$  diagonal elements of the density matrix by decreasing value, such that  $p_0$  is the largest, and  $p_{2^n-1}$  is the smallest.

Written in terms of  $\varepsilon$ , the reset step has the effect of changing the traced density matrix of the reset spin to

$$\rho_\varepsilon = \frac{1}{e^\varepsilon + e^{-\varepsilon}} \begin{pmatrix} e^\varepsilon & \\ & e^{-\varepsilon} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 + \varepsilon_0 & \\ & 1 - \varepsilon_0 \end{pmatrix}, \quad (40)$$

for any previous state. From eq 40 it is clear that  $\varepsilon_0 = \tanh \varepsilon$  as stated in the introduction. For a single spin in any diagonal mixed state:

$$\begin{pmatrix} p_0 \\ p_1 \end{pmatrix} \xrightarrow{RESET} \frac{p_0 + p_1}{2} \begin{pmatrix} 1 + \varepsilon_0 & \\ & 1 - \varepsilon_0 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 + \varepsilon_0 & \\ & 1 - \varepsilon_0 \end{pmatrix}. \quad (41)$$

For two spins in any diagonal state a reset of the least significant bit results in

$$\begin{pmatrix} p_0 \\ p_1 \\ p_2 \\ p_3 \end{pmatrix} \xrightarrow{RESET} \frac{p_0 + p_1}{2} \begin{pmatrix} \frac{p_0 + p_1}{2}(1 + \varepsilon_0) & & & \\ & \frac{p_0 + p_1}{2}(1 - \varepsilon_0) & & \\ & & \frac{p_2 + p_3}{2}(1 + \varepsilon_0) & \\ & & & \frac{p_2 + p_3}{2}(1 - \varepsilon_0) \end{pmatrix}. \quad (42)$$

Algorithm 6 may be highly inefficient in terms of logic gates. Each SORT could require an exponential number of gates. Furthermore, even calculation of the required gates might be exponentially hard.

We refer only to diagonal matrices and the diagonal elements of the matrices (applications of the gates considered here to a diagonal density matrix do not produce off-diagonal elements). For a many-spin system, RESET of the reset spin, transforms the diagonal of any diagonal density matrix,  $\rho$ , as follows:

$$Diag(\rho) = (p_0, p_1, p_2, p_3, \dots) \rightarrow \left[ \frac{p_0 + p_1}{2}(1 + \varepsilon_0), \frac{p_0 + p_1}{2}(1 - \varepsilon_0), \frac{p_2 + p_3}{2}(1 + \varepsilon_0), \frac{p_2 + p_3}{2}(1 - \varepsilon_0), \dots \right], \quad (43)$$

as the density matrix of each pair,  $p_i$  and  $p_{i+1}$  (for even  $i$ ) is transformed by the RESET step as described by eq 40 above. We use the definition of S&S probabilities,  $p' = 2^n(p - 2^{-n})/\varepsilon_0$ . The resulting S&S diagonal is

$$\begin{aligned} Diag(\rho') &= \left[ \frac{2^n}{\varepsilon_0} \left( \frac{p_0 + p_1}{2} + (1 + \varepsilon_0) - 2^{-n} \right), \dots \right] = \\ &= \left[ \frac{2^n}{\varepsilon_0} \left( \frac{p_0 + p_1}{2} - 2^{-n} \right) + 2^n \frac{p_0 + p_1}{2}, \dots \right] = \\ &= \left[ \frac{p'_1 + p'_2}{2} + 1, \frac{p'_0 + p'_1}{2} + 2^n \frac{p_0 + p_1}{2}, \frac{p'_0 + p'_1}{2} - 2^n \frac{p_0 + p_1}{2}, \dots \right], \end{aligned} \quad (44)$$

where the second element is shown in the final expression. We now use  $p = 2^{-n}(\varepsilon_0 p' + 1)$ , to obtain

$$2^n \frac{p_0 + p_1}{2} = 2^n \frac{2^{-n}(\varepsilon_0 p'_0 + 1) + 2^{-n}(\varepsilon_0 p'_1 + 1)}{2} \quad (45)$$

$$= \frac{\varepsilon_0(p'_0 + p'_1) + 2}{2} = 1 + \varepsilon_0 \frac{p'_0 + p'_1}{2}. \quad (46)$$

Ref [18] provides an analysis of the PPA. We continue, as in the previous subsection, to analyze the case of  $p'\varepsilon_0 \ll 1$ , which is of practical interest. In this case  $1 + \varepsilon_0 \frac{p'_0 + p'_1}{2} \approx 1$ . Hence, the effect of a RESET step on the S&S diagonal is:

$$Diag(\rho') = (p'_0, p'_1, p'_2, p'_3, \dots) \rightarrow \left[ \frac{p'_0 + p'_1}{2} + 1, \frac{p'_0 + p'_1}{2} - 1, \frac{p'_2 + p'_3}{2} + 1, \frac{p'_2 + p'_3}{2} - 1, \dots \right] \quad (47)$$

Consider now three spins, such that the one at the right is a reset spin. Following ref [18], we initially apply the PPA to three spins which are initially at the completely mixed state. The first step of the PPA, RESET (eq 47), is applied to the diagonal of the completely mixed state (eq 33), to yield

$$Diag(\rho'_{CMS}) \rightarrow Diag(\rho'_{RESET}) = (1, -1, 1, -1, 1, -1, 1, -1). \quad (48)$$

This diagonal corresponds to the density matrix

$$\rho_{RESET} = \frac{1}{2^3} \mathcal{I} \otimes \mathcal{I} \otimes \begin{pmatrix} 1 + \varepsilon_0 & \\ & 1 - \varepsilon_0 \end{pmatrix}, \quad (49)$$

namely to the bias configuration  $\{0, 0, \varepsilon_0\}$ . The next PPA step, SORT, sorts the diagonal elements in decreasing order:

$$Diag(\rho'_{SORT}) = (1, 1, 1, 1, -1, -1, -1, -1), \quad (50)$$

that arises from the density matrix

$$\rho_{SORT} = \frac{1}{2^3} \begin{pmatrix} 1 + \varepsilon_0 & \\ & 1 - \varepsilon_0 \end{pmatrix} \otimes \mathcal{I} \otimes \mathcal{I}, \quad (51)$$

which corresponds to the biases  $\{\varepsilon_0, 0, 0\}$ . The bias was thus transferred to the leftmost spin. In the course of repeated alternation between the two steps of the PPA, this diagonal will further evolve as detailed in Example 12.

The rightmost column of Example 12 lists the resulting bias configurations. Notice that after the 5<sup>th</sup> step the biases are identical. Also notice that in the 6<sup>th</sup> and 10<sup>th</sup> steps the states  $|100\rangle$  and  $|011\rangle$  are exchanged (3B-Comp); after both these steps, the state of the system cannot be written as a tensor product.<sup>6</sup> Also notice that after step 13, the PPA applies a SORT which will also switch between these two states. The PPA, applied to the bias configuration  $\{t\varepsilon_0, \varepsilon_0, \varepsilon_0\}$ , where  $1 \leq t \leq 2$  is simply an exchange  $|100\rangle \leftrightarrow |011\rangle$ . This is evident from the diagonal

$$Diag(\rho') = (t + 2, t, t, t - 2, -t + 2, -t, -t, -t - 2). \quad (52)$$

Thus, the PPA on three spins is identical to the Fibonacci algorithm applied to three spins (see Example 6). This analogy may be taken further to some extent. When the PPA is applied onto four spins, the outcome, but not the steps, is identical to the result obtained by Tribonacci algorithm (see Example 8). These identical results may be generalized to the PPA and all-bonacci applied onto  $n \geq 3$  spins.

**Example 12:** *Application of PPA to 3 spins*

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<sup>6</sup> This is due to *classical* correlations (not involving entanglement) between the spins; an individual bias may still be associated with each spin by tracing out the others, but such a bias cannot be interpreted as temperature.



	$Diag(\rho') = (0, 0, 0, 0, 0, 0, 0, 0)$	$\{0, 0, 0\}$
step 1	$\xrightarrow{RESET} (1, -1, 1, -1, 1, -1, 1, -1)$	$\{0, 0, \varepsilon_0\}$
step 2	$\xrightarrow{SORT} (1, 1, 1, 1, -1, -1, -1, -1)$	$\{\varepsilon_0, 0, 0\}$
step 3	$\xrightarrow{RESET} (2, 0, 2, 0, 0, -2, 0, -2)$	$\{\varepsilon_0, 0, \varepsilon_0\}$
step 4	$\xrightarrow{SORT} (2, 2, 0, 0, 0, 0, -2, -2)$	$\{\varepsilon_0, \varepsilon_0, 0\}$
step 5	$\xrightarrow{RESET} (3, 1, 1, -1, 1, -1, -1, -3)$	$\{\varepsilon_0, \varepsilon_0, \varepsilon_0\}$
step 6	$\xrightarrow{SORT} (3, 1, 1, 1, -1, -1, -1, -3)$	$N. A.$
step 7	$\xrightarrow{RESET} (3, 1, 2, 0, 0, -2, -1, -3)$	$\{\frac{3\varepsilon_0}{2}, \frac{\varepsilon_0}{2}, \varepsilon_0\}$
step 8	$\xrightarrow{SORT} (3, 2, 1, 0, 0, -1, -2, -3)$	$\{\frac{3\varepsilon_0}{2}, \varepsilon_0, \frac{\varepsilon_0}{2}\}$
step 9	$\xrightarrow{RESET} \frac{1}{2}(7, 3, 3, -1, 1, -3, -3, -7)$	$\{\frac{3\varepsilon_0}{2}, \varepsilon_0, \varepsilon_0\}$
step 10	$\xrightarrow{SORT} \frac{1}{2}(7, 3, 3, 1, -1, -3, -3, -7)$	$N.A.$
step 11	$\xrightarrow{RESET} \frac{1}{2}(7, 3, 4, 0, 0, -4, -3, -7)$	$\{\frac{7\varepsilon_0}{4}, \frac{3\varepsilon_0}{4}, \varepsilon_0\}$
step 12	$\xrightarrow{SORT} \frac{1}{2}(7, 4, 3, 0, 0, -3, -4, -7)$	$\{\frac{7\varepsilon_0}{4}, \varepsilon_0, \frac{3\varepsilon_0}{4}\}$
step 13	$\xrightarrow{RESET} \frac{1}{4}(15, 7, 7, -1, 1, -7, -7, -15)$	$\{\frac{7\varepsilon_0}{4}, \varepsilon_0, \varepsilon_0\}$

## 4 Optimal Algorithmic Cooling

### 4.1 Lower Limits of the PPA and All-bonacci

Consider an application of the PPA to a three-spin system at a state with the S&S diagonal of eq 37. This diagonal is both sorted and invariant to RESET, hence it is invariant to the PPA. Eq 37 corresponds to the bias configuration  $\{2\varepsilon_0, \varepsilon_0, \varepsilon_0\}$  which is the limit of the Fibonacci algorithm presented above (eq 12). This configuration is the “lower” limit of the PPA with three spins in the following sense: any “hotter configuration” is not invariant and continues to cool down during exhaustive PPA until reaching or bypassing this configuration. For four spins the diagonal of Eq 38 is invariant to the PPA for the same reasons. This diagonal corresponds to the bias configuration  $\{4\varepsilon_0, 2\varepsilon_0, \varepsilon_0, \varepsilon_0\}$ , which is the limit of the Tribonacci algorithm (or the all-bonacci) applied to four spins. Any “hotter configuration” is not invariant and cools further during exhaustive PPA, until it reaches (or bypasses) this configuration.

Now, we follow the approximation of very small biases for  $n$  spins, where  $2^n \varepsilon_0 \ll 1$ . The diagonal in eq 39 is invariant to the PPA. This diagonal corresponds to the bias configuration

$$\{2^{n-2}\varepsilon_0, 2^{n-3}\varepsilon_0, 2^{n-4}\varepsilon_0, \dots, 2\varepsilon_0, \varepsilon_0, \varepsilon_0\}, \quad (53)$$

which is the limit of the all-bonacci algorithm. As before, any “hotter configuration” is not invariant and cools further. It is thus proven that the PPA reaches at least the same biases as all-bonacci.

We conclude that under the assumption  $2^n \varepsilon_0 \ll 1$ , the  $n$ -spin system can be cooled to the bias configuration shown in eq 53. When this assumption is not valid (e.g., for larger  $n$  with the same  $\varepsilon_0$ ), pure qubits can be extracted; see theorem 2 in [19] (theorem 3 in ref [18]).

Yet, the PPA potentially yields “colder configurations”. We obtained numerical results for small spin systems which indicate that the limits of the PPA and all-bonacci are identical. Still, since the PPA may provide better cooling, it is important to put an “upper” limit on its cooling capacity.

### 4.2 Upper Limits on Algorithmic Cooling

Theoretical limits for cooling with algorithmic cooling devices have recently been established [18,19]. For any number of reset steps, the PPA has been shown to be optimal in terms of entropy extraction (see ref [19] and more details in section 1 of ref [18]). An upper bound on the degree of cooling attainable by the PPA is therefore also an upper bound of any AC algorithm. The following theorem regards a bound on AC which is the loose bound of ref [18].

**Theorem 1** *No algorithmic cooling method can increase the probability of any basis state to above<sup>7</sup>  $\min\{2^{-n}e^{2^n\varepsilon}, 1\}$ , where the initial configuration is the completely mixed state.<sup>8</sup> This includes the idealization where an unbounded number of reset and logic steps can be applied without error or decoherence.*

The proof of Theorem 1 involves applying the PPA and showing that the probability of any state never exceeds  $2^{-n}e^{2^n\varepsilon}$ .

## 5 Algorithmic Cooling and NMR Quantum Computing

We have been using the language of classical bits, however spins are quantum systems; thus, spin particles (two-level systems) should be regarded as quantum bits (qubits). A molecule with  $n$  spin nuclei can represent an  $n$ -qubit computing device. The quantum computing device in this case is actually an ensemble of many such molecules. In ensemble NMR quantum computing [20,21,22] each computer is represented by a single molecule, such as the TCE molecule of Fig. 1, and the qubits of the computer are represented by nuclear spins. The macroscopic number of identical molecules available in a bulk system is equivalent to many processing units which perform the same computation in parallel. The molecular ensemble is placed in a constant magnetic field, so that a small majority of the spins are aligned with the direction of the field. To perform a desired computation, the same sequence of external pulses is applied to all molecules/computers. Any quantum logic-gate can be implemented in NMR by a sequence of radio-frequency pulses and intermittent delay periods during which spins evolve under coupling [23]. Finally, the state of a particular qubit is measured by summing over all computers/molecules. The process of AC constitutes a simple quantum computing algorithm. However, unlike other quantum algorithms, the use of quantum logic gates does not produce any computational speed-up, but instead generates colder spins. This constitutes the first near-future application of quantum computing devices. AC may also have an important long-term application; it may enable quantum computing devices capable of running important quantum algorithms, such as the factorization of large numbers [24]. NMR quantum computers [20,21,22] are currently the most successful quantum computing devices (see for instance ref [25]), but are known to suffer from severe scalability problems [1,26,27]. AC can be used for building scalable NMR quantum computers of 20-50 quantum bits if electron spins are used for the PT and RESET steps. PT with electron spins [9,11] can enhance the polarization by three or four orders of magnitude. Unfortunately, severe technical difficulties have thus far impeded common practice of this technique. An example of such a difficulty is the need to master two very different electromagnetic frequencies within a single machine. However, in case such PT steps come into practice (using machinery that allows conventional NMR techniques as well), AC could be applied with much better parameters; First,  $\varepsilon_0$  could be increased to around 0.01-0.1. Second, the ratio  $R_{\text{relax-times}}$  could reach  $10^3 - 10^4$ . With these figures, scalable quantum computers of 20-50 qubits may become feasible.

## 6 Discussion

Algorithmic Cooling (AC) harnesses the environment to enhance spin polarization much beyond the limits of reversible polarization compression (RPC). Both cooling methods may be regarded as a set of logic gates, such as NOT or SWAP, which are applied onto the spins. Polarization transfer (PT), for instance, a form of RPC, may be obtained by a SWAP gate. AC algorithms are composed of two types of steps: reversible AC steps (RPC) applied to two spins or more, and reset steps, in which entropy is shifted to the environment through reset spins. These reset spins thermalize much faster than computation spins (which are cooled), allowing a form of a molecular heat pump. A prerequisite for AC is thus the mutual existence (on the same molecule) of two types of spins with

<sup>7</sup> A tighter bound,  $p_0 \leq 2^{-n}e^{2^{n-1}\varepsilon}$ , was claimed by theorem 1 of ref [18].

<sup>8</sup> It is assumed that the computation spins are initialized by the polarization of the reset spins.

a substantial relaxation times ratio (of at least an order of magnitude). While this demand limits the applicability of AC, it is often met in practice (e.g., by  $^1\text{H}$  vs  $^{13}\text{C}$  in certain organic molecules) and may be induced by the addition of a paramagnetic reagent. The attractive possibility of using rapidly-thermalizing electron spins as reset bits is gradually becoming a relevant option for the far future.

We have surveyed previous cooling algorithms and suggested novel algorithms for exhaustive AC: the Tribonacci, the  $k$ -bonacci, and the all-bonacci algorithms. We conjectured the optimality of all-bonacci, as it appears to yield the same cooling level as the PPA of refs [18,19]. Improving the SNR of NMR by AC potentially constitutes the first short-term application of quantum computing devices. AC is further accommodated in quantum computing schemes (NMR-based or others) relating to the more distant future [1,28,29,30].

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